

Present: John Straub, Ken Jordan, Bruce Kay, Sharon Hammes-Schiffer, Rod Bartlett, Susan Tucker, Krishnan Raghavachari, Jan Steckel, and Martin Head-Gordon

Items Discussed:

1. To whom theory subdivision location information should be sent: all present and past officers of the subdivision as well as current chair of biophysical subdivision, Chair of Comp Division (currently Wendy Cornell) P-chem program chairs.
2. New officers: Angel Garcia is Vice Chair and Krishnan Raghavachari is Chair Elect, Secretary is Jan Steckel.
3. Newsletter was last published 2002. Should be resurrected in electronic form. Secretary will prepare the newsletter, containing summaries of the symposia as well as announcements and send e-mail to all theory subdivision members with link to newsletter, which would be on the web page. Information on the newsletter will strongly overlap with information currently on the web page but that's ok because the newsletter will become a sort of archive for the subdivision.
4. How does information for the web page get to John Adams? Secretary will contact him to coordinate web-hosting for the newsletter and find out if there is any other information about the subdivision he needs.
5. Post-doc and/or faculty positions posted on web page? Is this a lot of work for the web master? Are there other clearing houses for this purpose (OSU comp chemistry list)?
6. Posting of upcoming meetings and workshops (significant theory content) on web page and newsletter. Organizers of upcoming meetings should be invited to send information to John Adams.
7. Should the subdivision do a formal or informal survey of its members to find out a) do they want a newsletter b) what should be in it c) do they care to read summaries of the symposia d) do they want the subdivision webpage or newsletter to serve as a clearinghouse for post-doc and/or faculty openings? The idea was discussed but not positively adopted.
8. ACS mailing lists were discussed at the meeting and questions arose about it. Since the meeting, Elaine Springle provided the following information regarding the mailing lists. ACS sends lists, containing e-mail (not guaranteed to be current) for Theory subdivision members about four times per year to Elaine. Secretary should contact ACS to find out about having those lists sent directly or just get them from Elaine.
9. Question arose as to whether theory subdivision mailing list should be made available to others who request it; consensus was probably not.
10. Question arose as to how one formally joins the subdivision; does a candidate notify subdivision secretary or sign up directly with ACS. This may have changed. Secretary will look into this so that our next newsletter contains correct 'instructions' as to how to become a member.
11. IBM award has been resurrected for a one-year commitment only; award is \$3,500. There used to be a grant of computer time with the award; currently there is none and to make it worthwhile, it would need to be a lot more significant than what used to be given. If computer time was sought, it should be on IBM computers. Jamie Coffin and Bill Swope at IBM will be involved in the awards process and they would like to see parallel processing or grid processing. The award should be advertised on the JPC website and of course our webpage and newsletter.
12. Proposed symposia were discussed. In terms of the symposium proposed by Jianshu Cao, "Advances in condensed phase quantum dynamics: Theory and new applications", we suggested that he focus it more and avoid repetition of the topics covered in the two recent quantum/classical symposia in fall 2003 and spring 2004. It was suggested that there be one quantum chemistry symposium per year since it is a very active field. Krishnan suggested the symposium "Quantum Chemistry of complex systems" (or some other similar variation) for 2006. This will complement the symposium in Fall 2005 which is more focused on smaller systems.